NIH ANNUAL REPORT RR-612 1/1/73 - 12/31/73

## ANNUAL REPORT FOR RESEARCH PROJECT: "RESOURCE RELATED RESEARCH -- COMPUTERS AND CHEMISTRY" LIH GRANT 5 R24 RROO612-03

## TABLE OF CONTENTS

			<u>Page</u>
Ι.	App	clication For Continuation	1
IT.	Progress Report		
	Α.	Applications of Artificial Intelligence to Mess Spectrometry	2
	В.	Extensions of the Computer-Mass Spectrometry System	10
	С.	Extending the Theory of Mass Spectrometry by a Computer	24
II.	Sig	nature of Principal Investigator	28
IV.	Resource Finances		
	Α.	Summary of Resource Expenditures	29
	R	To additure Details - Addounts A, B & C	30
		1. Budget Explanation - Justification	33
	C.	Estimate - Next Budget Period	34
		1. Budget Explanation - Justification	38
	D.	Supporting Data for Administrative Extension	3,-
	Appendix		
	Α.	"Applications of Artificial Intelligence for Chemical Inference XI"	L
	В.	"Applications of Artificial Intelligence for Chemical Inference IX. Analysis of Mixtures Without Prior Separation as Illustrated for Estrogens"	
	С.	"Mass Spectrometry in Structural and Stereochemical ECCXXII. Delineation of Competing Fragmentation Pathy Complex Molecules from a Study of Metastable Jon " of Peuterated Derivatives"	to aysv

## Table of Contents, Cont'd.

- D. "Mass Spectrometry in Structural and Stereochemical Problems, CCXXXIV. Applications of DADI, a Technique for Study of "tetastable Ions, to Mixture Analysis"
- E. "Mass Spectrometry in Structural and Stereochemical Problems, CCXXXVIII. The Effect of Heteroatoms upon the Mass Spectrometric Fragmentation of Cyclohexanones"
- F. "Applications of Artificial Intelligence for Chemical Inference XII. Exhaustive Generation of Cyclic and Acyclic Isomers"
- G. "Applications of Artificial Intelligence for Chemical Inference XIII. Labelling Objects Having Symmetry"
- H. "Heuristic DENDRAL: Analysis of Molecular Structures"
- I. "Computer Generation of Vertex Graphs"
- J. "The Quantitation of BAIB in Urine by Mass Fragment graphy"
- K. "The Determination of Phenylalanine in Serum by Mass Fragmentography"
- L. "The Simultaneous Quantitation of Ten Amino Acids in Soil Extracts by Mass Fragmentography"
- M. "An Analysis of Twelve Amino Acids in Biological Fluids by Mass Fragmentography"
- N. "The Quantitation of B-Amino Isobutyric Acid in Urine by Mass Fragmentography"
- O. "The Determination of Ethanol in Blood and Urine by Mass Fragmentography"
- P. "A Study of the Electron Impact Fragmentation of Promazine Sulphoxide and Promazine using Specifically Deuterated Analogues"
- Q. "Mass Spectrometry in Structural and Stereochemical Problems. CCXXXVII. Electron Impact Induced Hydrogen Losses and Mignations in Some Aromatic Amides"
- P. "Spectrometrie de Masse. IX. Fragmentations Induites par Impact Electronique de Glycols-\alpha-En Serie Tetraline"
- S. "Spectrometrie de Masse. VIII. Elimination d'can Induite par Impact Electronique dans Le Tetrahydro-1,2,3,4-Napthtal-ene-diol-1,2"
- T. "Chlorination Studies I. The Reaction of Aqueous Hypochloreus Acid with Cytosine"

## Table of Contents, Cont'd.

- U. "Chlorination Studies II. The Reaction of Aqueous Hypochlorous Acid with ✓-Amino Acids and Dipeptides"
- V. "Chlorination Studies IV. The Reaction of Aqueous Hypochlorous Acid with Pyrimidine and Purine Bases"
- W. "Applications of Artificial Intelligence for Chemical Inference X. INTSUM. A Data Interpretation Program as Applied to the Collected Mass Spectra of Estrogenic Steroids"
- X. "Analysis of Behavior of Chemical Molecules: Rule Formation on Non-Homogeneous Classes of Objects"